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Measurements of hyperfine structure in Ta II

V. O. Zilio[1] and J. C. Pickering[2]★

[1]*Institute of Nuclear Engineering, Swiss Federal Institute of Technology, 1015, Lausanne, Switzerland*
[2]*Blackett Laboratory, Imperial College, London SW7 2BZ*

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ABSTRACT

We report the first extensive measurements of hyperfine structure in Ta II. Spectra of Ta II were recorded by high-resolution Fourier transform spectrometry in the region 10 000–53 000 cm^{-1} (1886–10 000 Å) and the majority of observed lines show significant hyperfine structure. Computer fits to several hundred of these line profiles have yielded values of the magnetic dipole hyperfine interaction constant A for 88 energy levels with an uncertainty of between 0.5 and 10 per cent for the majority of A factors. The A factors range from -0.078 to $+0.065$ cm^{-1} for the even levels and from -0.064 to $+0.083$ cm^{-1} for the odd levels. For the majority of these A factors no previous measurements are known. Approximate values of the electric quadrupole hyperfine interaction constant B were found for 73 levels. These measurements of A and B factors allow, for the first time, the effects of hyperfine structure in Ta II lines to be correctly accounted for both in abundance analysis and in the resolution of blended lines in astrophysical spectra.

Key words: atomic data – line: profiles.

1 INTRODUCTION

Knowledge of hyperfine structure (hfs) is essential in fitting of astrophysical spectra, in spectrum synthesis and abundance determinations. Hyperfine structure of Ta II levels is of interest particularly in studies of chemically peculiar stars (Henderson et al. 1999; Norquist & Beck 2001). With the new generation of high-resolution spectrographs on both ground and space-based telescopes hyperfine structure data is needed to correctly interpret line profiles, and to carry out accurate abundance determinations. In the analysis of the spectrum of chemically peculiar star χ Lupi (Leckrone et al. 1999) Ta II is listed in a table of ions needing more study. Experimental measurements of hfs for the ground level of Ta II exist: Brown & Tomboulian (1952) had measured seven lines of Ta II to determine hfs splitting of the ground level, and used this to calculate the magnetic moment and quadrupole moment. However, despite the need for hfs data for Ta II no comprehensive set of measurements were available prior to our work. The technique of Fourier transform (FT) spectroscopy is ideal for the analysis of hyperfine structure since its large free spectral range is combined with high resolution (Pickering 1996). FT spectroscopy therefore has many advantages over other accurate techniques such as those of the Fabry–Perot, or laser spectroscopy because with FT spectroscopy many hundreds or thousands of lines may be recorded in one scan with Doppler-limited resolution. An example of a hyperfine structure pattern observed by FT spectroscopy is shown in Fig. 1.

★E-mail: j.pickering@ic.ac.uk

2 EXPERIMENTAL DETAILS

The spectra used in this work were obtained using the UV Fourier Transform Spectrometer (FTS) at Imperial College, London (Thorne et al. 1987). The light source was a water-cooled hollow cathode lamp with a pure tantalum cathode. The lamp was run in either argon or neon as filler gases. The pressure used was about 0.4 mbar and the current was 300 mA. Argon was used as filler gas in the region 15 000–53 000 cm^{-1}, and neon was used in the 10 000–15 000 cm^{-1} region of the spectrum. Scans were recorded with a resolution of 0.036 cm^{-1}, and 16 coadded interferograms were combined to give a spectrum in each wavelength region. A variety of detectors (Hamamatsu photomultiplier tubes) and filters were used and these are listed in Table 1.

Tungsten and deuterium standard lamps were used to determine the instrument response, and thus provided intensity calibration. Lines from the tantalum spectra were investigated to find the hyperfine structure splitting factors (see Section 3). These spectra are also being analysed in an ongoing collaborative project with L. Windholz of Graz University and G. Guthöhrlein of the Universität der Bundeswehr Hamburg involving term analysis of Ta I and Ta II, and hfs in Ta I. Transitions of Ta I and Ta II are seen in the observed spectra together with lines of the particular filler gas, Ne or Ar. The line identifications and energy levels resulting from

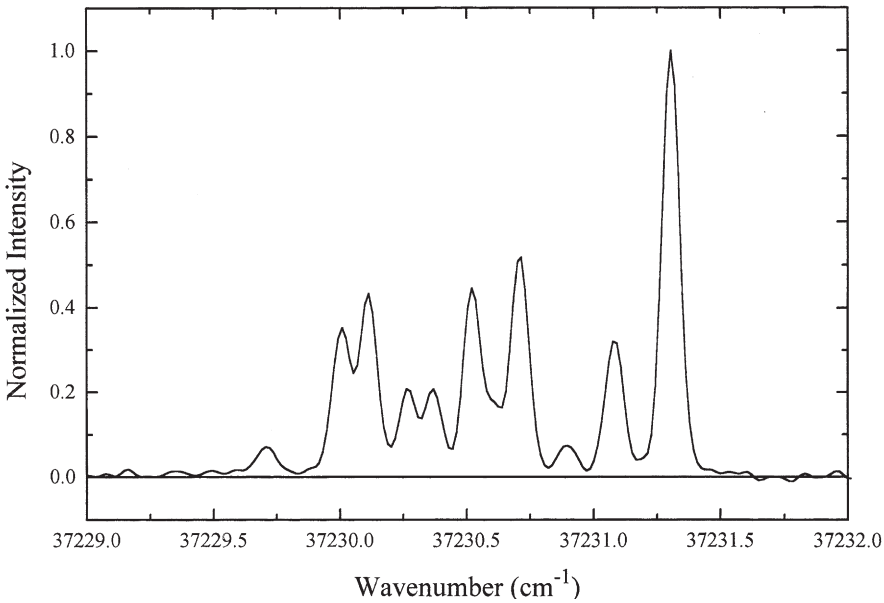

Figure 1. The line profile observed by Fourier Transform spectroscopy of the 2685 Å, 37 230.8 cm^{-1}, Ta II transition.

Table 1. Detectors (Hamamatsu photomultiplier tubes) and filters used in acquisition of spectra.

wavenumber range (cm^{-1})	detector	filter
9000–18 000	R928	LP665
11 000–23 000	R928	LP540
15 000–31 000	1P28	LP390
23 000–47 000	1P28	UG5
31 000–53 000	R166	–

the collaborative analysis project could be used to identify the Ta II lines studied in this paper.

3 HYPERFINE STRUCTURE ANALYSIS

3.1 Simple theory

For atoms with non-zero nuclear spin I the fine structure levels undergo splitting because of the hyperfine interaction between the nucleus and the electrons. In the absence of perturbations the energy of the hyperfine structure multiplets is given (Kopfermann 1958) by

$$W_F = W_J + \frac{1}{2}AK + B\frac{(3/4)K(K+1) - J(J+1)I(I+1)}{2I(2I-1)J(2J-1)}, \qquad (1)$$

where W_J is the energy of the fine structure level of quantum number J, A and B are the magnetic dipole and the electric quadrupole hyperfine interaction constants respectively, and K is defined as

$$K = F(F+1) - J(J+1) - I(I+1)$$

in which F is the quantum number associated with the total angular momentum of the atom,

$$F = I + J; \quad I + J - 1; \quad \ldots \quad ; |I - J|.$$

The selection rules which govern the hyperfine transitions are

$$\Delta F = 0; \pm 1 \quad \text{but not} \quad F = 0 \leftrightarrow F = 0.$$

In addition there are intensity rules (Kuhn 1962): within a hyperfine multiplet the ratio of the sums of the intensities of all transitions from two states with quantum numbers F and F' are in the ratio of their statistical weights $(2F + 1) : (2F' + 1)$.

This simple theory was used in the fitting of hfs of the Ta II transitions observed this work. No perturbations were evident.

3.2 Analysis of observed line profiles

The determination of the A and B factors for the Ta II energy levels was carried out using a hfs analysis subroutine (Pickering 1996) incorporated into the spectral analysis program, DECOMP (Brault & Abrams 1989). The input information comprises the I-value (7/2 for tantalum), the J-values of both levels, the known intensity ratios of the transition components (Kuhn 1962), the widths of the components (having Gaussian and Lorentzian contributions), and the centre-of-gravity of the line pattern. Using this fitting routine to analyse the transition line patterns, values for the magnetic dipole hyperfine interaction constant A were found for 88 levels of which the majority had previously unmeasured A factors. It was not always possible to determine the electric quadrupole hyperfine interaction constant B because the contribution of the last term in equation (1) was so small, but approximate B factors were found for 73 levels.

Any blends in observed lines were clearly discernable since either it was not possible to obtain a fit to the line profile or the line fitting process gave very large residual errors and A factors which were not consistent with values determined for the particular level from fits of other lines.

The values determined for A and B are listed in Table 2. The first two columns give, for each level investigated, the energy level

Table 2. Hfs interaction constants of the energy levels of Ta II.

Energy Level (cm^{-1})	J	A (mK)	A err (mK)	No. of Lines	B (mK)	B err (mK)
0.00	1	−78.2	0.5	11	−22	8
1031.33	2	34.4	0.5	18	−15	8
2642.19	3	45.5	0.5	19	−25	10
3180.04	2	19.7	0.5	8	13	5
4124.77	0	0.0			0	
4415.70	4	47.2	0.5	9	−25	8
5330.66	1	32.5	1.0	10	12	6
5658.00	2	48.3	0.5	11	−23	10
6186.72	5	48.5	0.5	7	−47	5
6831.35	3	11.8	0.5	7	45	10
9690.46	2	41.6	0.5	7	−27	5
9746.33	4	10.1	0.5	7	56	8
11767.14	3	−19.6	0.5	5	25	8
11875.46	2	65.3	0.5	4	−55	8
12435.85	3	64.4	3.0	1	0	10
12600.87	0	0.0			0	
12705.32	4	−17.0	0.5	2	62	5
12966.02	4	50.0	5	1	–	
13560.25	2	22.0	4	2	18	20
14158.52	5	47.0	5	1	95	40
14494.90	2	−9.0	3	2	15	10
14581.00	3	−23.0	3	2	–	
14627.75	1	−55.0	3	1	−20	10
15726.06	3	−3.0	2	1	−80	20
15851.12	4	−22.0	2	4	33	10
16288.04	0	0.0			0	
17168.50	2	53.0	3	2	−10	10
23082.70	4	−12.0	3	1	−120	5
23294.70	2	14.0	4	3	60	8
23381.19	0	0.0			0	
29256.87	2	−18.2	0.5	3	30	5
32318.44	3	47.0	0.5	4	14	5
33706.50	1	−63.7	0.5	4	−14	5
33715.15	2	22.1	0.3	2	−50	5
36112.97	4	51.2	0.3	4	52	5
36177.12	2	15.4	0.5	3	–	
36763.73	3	42.1	0.3	2	−45	5
36987.73	1	74.0	0.3	4	−3	8
37230.80	2	41.4	1.0	3	–	
37395.96	0	0.0			0	
38515.55	2	19.7	0.5	3	3	5
38535.26	1	−53.9	0.3	3	−12	5
38962.38	3	35.8	0.5	2	−12	5
39295.83	3	32.3	0.5	2	75	5
39743.64	4	31.7	0.5	3	−35	5
40023.68	0	0.0			0	
40233.53	2	62.8	0.5	2	−30	15
40304.78	1	20.4	0.5	2	−25	5
41145.00	2	22.7	0.7	4	–	
41554.52	3	24.6	0.7	7	–	
41709.02	5	30.4	0.3	4	15	5
41775.29	4	29.4	0.5	2	65	5
42122.91	4	33.9	0.5	3	58	5
42153.32	2	0.4	0.5	5	25	8
42959.59	3	32.5	0.5	2	–	
43064.95	2	34.1	0.5	4	0	10
43068.72	0	0.0			0	
43544.44	3	6.1	0.5	8	32	8
43553.87	1	82.9	0.5	1	−10	5
44005.16	4	31.0	2	3	10	10
44206.19	1	40.0	8	1	−50	40
44259.20	2	42.0	3	3	−50	30
44430.38	3	23.0	2	4	80	40
44434.70	0	0.0			0	
44585.33	5	34.2	0.7	1	13	10
44626.00	4	36.0	3	3	60	40
44835.23	3	13.0	3	5	0	10
45233.85	1	42.0	3	2	−27	10
46023.76	0	0.0			0	
46174.63	1	56.0	7	1	–	
46295.07	5	22.0	1	1	8	5
46387.28	2	59.0	3	1	−30	20
46645.81	4	8.0	0.5	3	–	
46831.39	3	10.0	3	2	–	
46850.69	2	37.5	2	1	−50	30
47169.18	3	3.5	1	1	30	30
47280.92	4	12.6	0.5	3	35	8
47514.61	2	27.0	5	1	0	20
47596.62	1	0.5	3	1	–	
47800.95	0	0.0			0	
47825.41	3	30.0	3	3	−3	10
47830.00	6	4.8	0.3	1	81	5
48064.50	0	0.0			0	
48162.10	4	33.0	5	1	125	40
48470.35	4	25.0	2	2	22	8
48666.55	2	−32.5	0.5	1	62	10
48776.36	1	−2.5	2	1	25	20
48962.66	3	43.0	5	1	−65	40
49055.18	5	14.7	0.5	1	7	5
49080.44	2	−2.0	3	1	25	20
49646.60	3	5.5	3	1	25	20
50507.12	5	38.5	2	1	90	20
51073.88	3	12.9	0.5	4	−40	10
52155.76	1	7.0	6	1	0	40
53011.00	2	11.0	5	1	−5	40
53343.56	4	−28.0	6	1	25	20
54648.81	3	5.0	2	2	50	10
61694.17	3	−31.0	5	1	–	
64653.35	3	12.0	1	1	–	

Hyperfine structure A and B splitting factors for levels of Ta II. The energy levels are given by their energy value (italics indicates odd parity energy levels) and J value. The number of lines analysed to determine the A factor is given in column 5. A and B factors, together with their uncertainties, are given in mK, where $1\,\mathrm{mK} = 0.001\,\mathrm{cm}^{-1}$.

value (Moore 1958) and J-value. The third and fourth columns give the A factor and its uncertainty in mK ($1\,\mathrm{mK} = 0.001\,\mathrm{cm}^{-1}$) determined in this work. The next column gives the number of spectral lines that were fitted in order to determine the value of A. The final two columns list the approximate value of the B factor and its uncertainty. This analysis has been carried out based entirely on the spectral line profiles observed in this work. No previous measurements of A factors were used.

In general, for each level studied the hfs A factor was determined from the analysis of line profiles for between 3 and 6 different transitions, resulting in a range of A values usually differing by a fraction of 1 mK. The differences arise for several reasons: uncertainties in the A factor of the other level involved in a transition; a range of signal-to-noise ratios of observed lines; and differing Doppler line widths. Typical Doppler widths are 80 mK at $35\,000\,\mathrm{cm}^{-1}$, and 100 mK at $44\,000\,\mathrm{cm}^{-1}$. The resolution of the FT spectrometer is such that the line widths are limited solely by the Doppler widths and so, depending on the size of the A factors, the overall pattern is usually well resolved into individual components in the longer wavelength regions, but only partly so in the UV. However, even where a set of line profiles did not appear to be resolved into individual components, the fitting still gave consistent sets of A factors. In many cases A factors determined for a particular level from several transitions agreed to within 0.1 mK. The uncertainties listed in Table 2 are estimated from the range of values of each particular A factor. Hfs in Ta II is also being

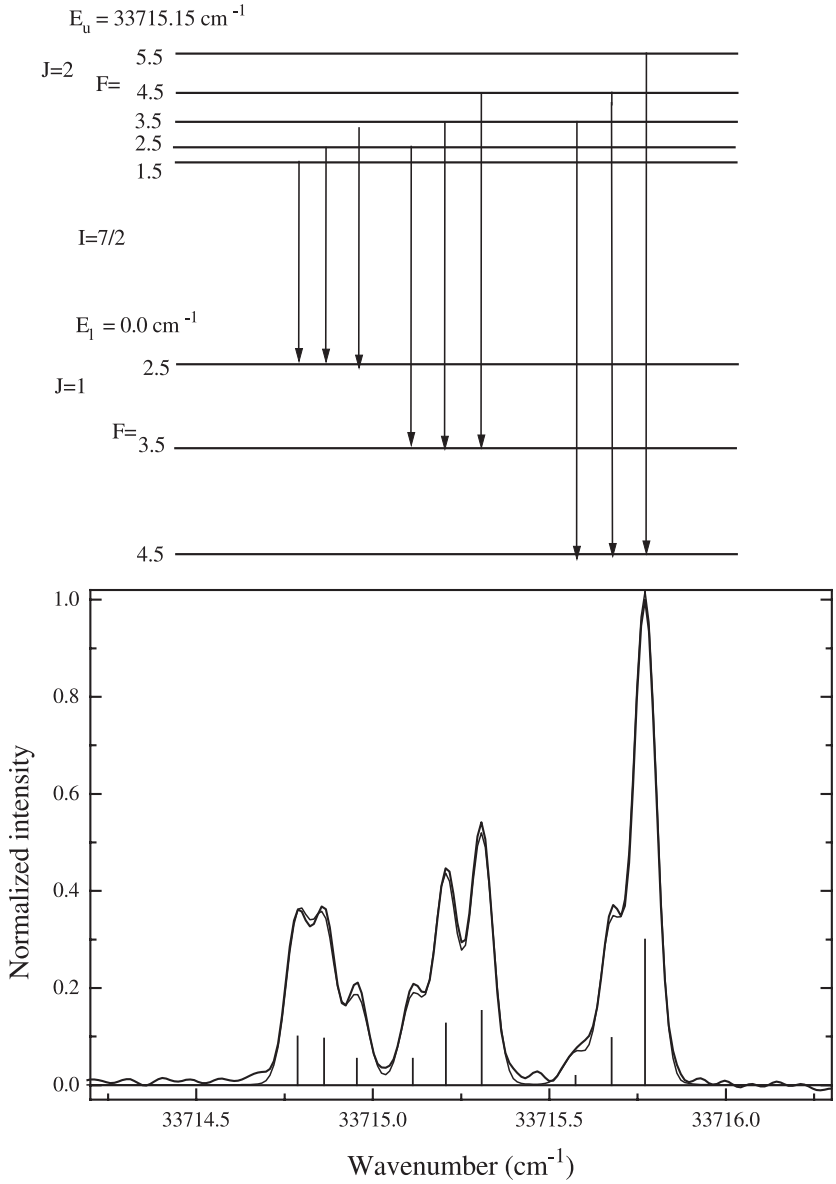

Figure 2. The observed (heavier trace in plot) and fitted line profiles, hyperfine components and transition diagram for the Ta II 33 715.15 cm^{-1} transition.

studied at the Universität der Bundeswehr Hamburg using the technique of laser-induced fluorescence detection to measure *A* and *B* factors for selected levels (Messnarz 2001) (Messnarz & Guthöhrlein 2002). Our results are in good agreement with this accurate technique.

When *B* factors could not be determined, because of poor signal-to-noise ratio of the investigated lines or poor resolution of the line components, they were removed from the fitting program. Setting $B = 0$ in line profile fits tended to give rise to greater variation in the *A* factors found for a particular level, and is reflected in the higher uncertainties given for *A* factors in this circumstance. In some cases the *B* factors determined from the line profile fitting of several transitions showed agreement to within 50 per cent and these values were considered to be meaningful; they should however be regarded as very approximate, and they are listed in Table 2. For the majority of analysed transitions of reasonable signal-to-noise ratio and exhibiting fairly well resolved hfs splitting the profiles could only be fitted by including both *A* and *B* factors in the fitting process. For these transitions if $B = 0$ was set in the line profile fit a large residual would result.

Examples of fitted line profiles together with schematic diagrams of the energy levels involved in the transitions are shown in Figs 2 and 3.

4 CONCLUSIONS

We present the first comprehensive set of measurements of hfs *A* and *B* splitting factors for singly ionized tantalum.

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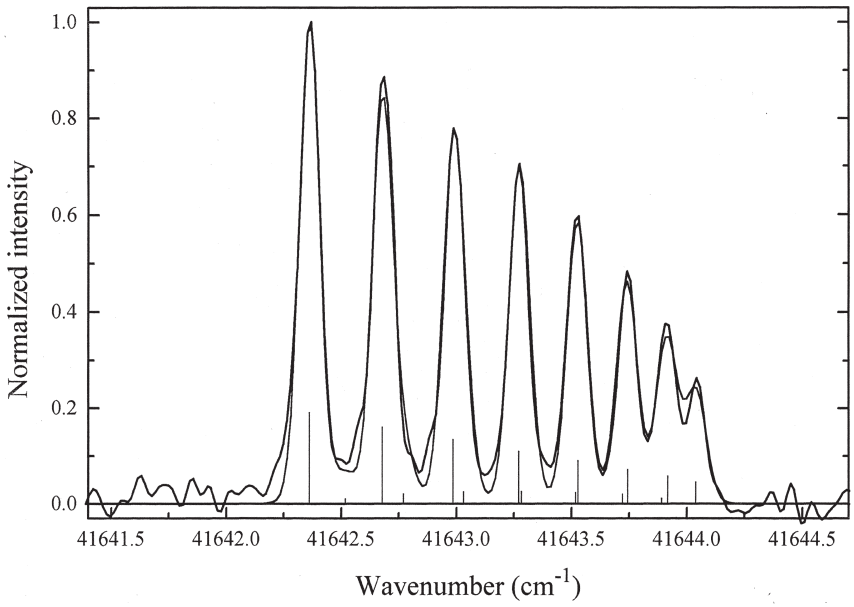

Figure 3. The observed (heavier trace in plot) and fitted line profiles, and hyperfine components for the Ta II 41 643.28 cm^{-1} transition.

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